

§24. Atomic and Molecular Data Compilation and Update of the NIFS Databases for Molecular Targets

Kimura, M. (Kyushu U.), Igarashi, A. (Miyazaki U.), Motohashi, M. (Tokyo U. Ag. and Tech.), Kusakabe, T. (Kinki U.), Morishita, T. (U. Elec-Comm.), Moribayashi, K. (JAEA), Kitajima, M. (Tokyo Inst. Tech.), Imai, M. (Kyoto U.), Pichl, L. (ICU.), Kato, D., Murakami, I., Kato, T.

Continuing and systematic efforts for making revision and update of NIFS databases have been carried out for electron and ion impacts on various atomic and some molecular targets by a few atomic and molecular collision physicists over the years by having obtained many participants. The original databases called AMIDIS for electron collisions and CHART for heavy-particle collisions, respectively, have been completed over decades ago, and from time to time, some efforts have been taken to update the databases by collecting those recently published, critically evaluating these data and implementing into these databases. Since the last revision made sometime ago, probably more reliable data for various atomic and molecular systems at different collision energy range are now available. Therefore, new and systematic effort to update these databases is considered to be not only important, but also indispensable to preserve human knowledge for future generations. In this contract year, we are concerned with molecular targets by electron and ionic impacts. For recent years, theoretically very extensive and accurate calculations have been performed routinely for inelastic processes for electronic and ionic impacts, while experimentally very elaborate beam experiments are also carried out, in combination with various types of lasers, so that one can determine different scattering parameters fairly accurately. Consequently,

significant progress for both areas has been made particularly since 1990. Therefore, we have felt it essential to reevaluate these new data critically and establish recommended values for electron and heavy-particle ionic impacts for molecular targets in the NIFS databases.

Electron impact:

Compilation of the cross sections for the electron-impact excitation and ionization of various molecules such as hydrocarbons was attempted. With the close collaboration with specialists in the plasma-processing community, we have also undertaken the systematic effort to collect cross-section data for those molecular targets relevant to plasma processing such as C_mF_n and C_mCl_n . In addition, some attempts have been made to collect and evaluate cross-section data for ionic species. Extensive and systematic calculations based on the R-matrix method were performed recently for ionic targets by one of our members, and the cross section data from these studies were included in AMDIS.

Ion impact:

For ion impact, we have reviewed H^+ , B^{q+} (where $q = 1-5$), and C^{q+} ($q = 1-6$) impacts on hydrocarbons and other common molecules such as O_2 , H_2O , and CO_2 from keV to meV collision energies, although very little investigation has been carried out for molecular targets. We have initiated a joint experimental and theoretical investigation to produce and evaluate cross section data for molecular targets by ion impact. This year, we have primarily been concerned with larger hydrocarbons such as C_mH_n where $m > 2$ and $n > 4$.

Based on these investigations, we have completed a report of the progress of our activity which will be published as a NIFS report in 2006. Another report will be published as a regular article in *Journal of Physical and Chemical Data*.